

## Supplementary Materials:

### 1. Mass spectra of the Schiff bases 1, 2 and 3

The mass spectra showed ion peak at  $m/z = 270.11$  as the molecular ion peak ( $[M+H]^+$ ) of Schiff base **1** (Fig. S1). The ion peak at  $m/z = 320.13$  is due to the molecular ion peak ( $[M+H]^+$ ) of Schiff base **2** (Fig. S2). The ion peak at  $m/z = 300.12$  corresponds to the molecular ion peak ( $[M+H]^+$ ) of Schiff base **3** (Fig. S3). The above results are consistent with the theoretical molecular weight of Schiff base **1** ( $C_{16}H_{15}NO_3$ : Mr = 269.30), Schiff base **2** ( $C_{20}H_{17}NO_3$ : Mr = 319.36) and Schiff base **3** ( $C_{17}H_{17}NO_4$ : Mr = 299.32), respectively.

#### Schiff base 1

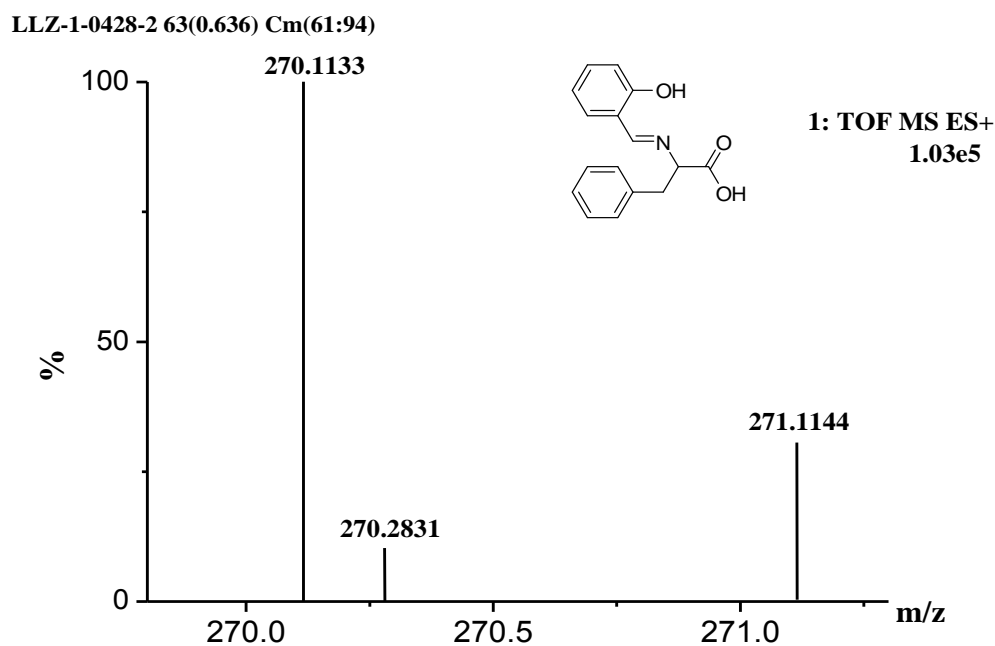
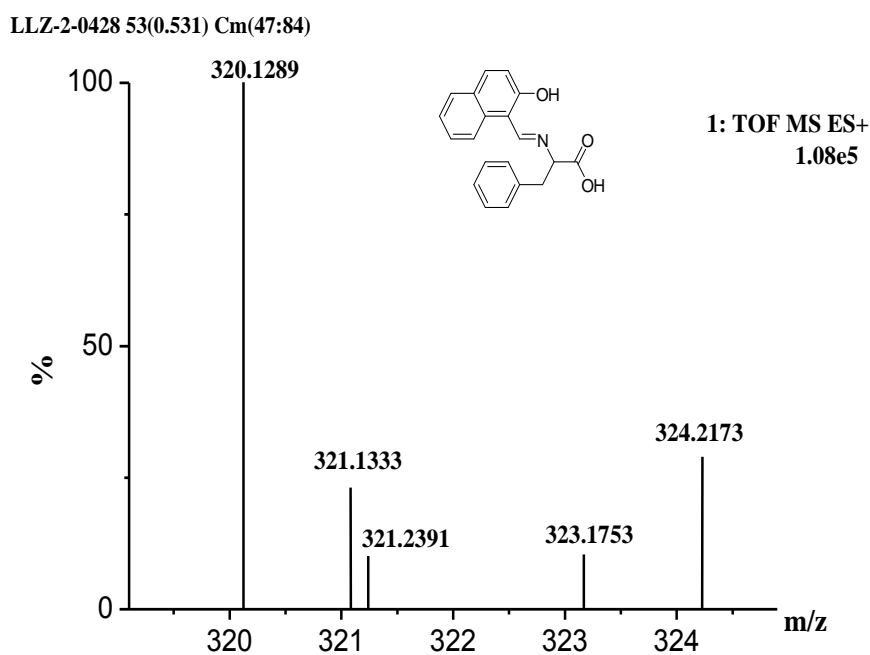


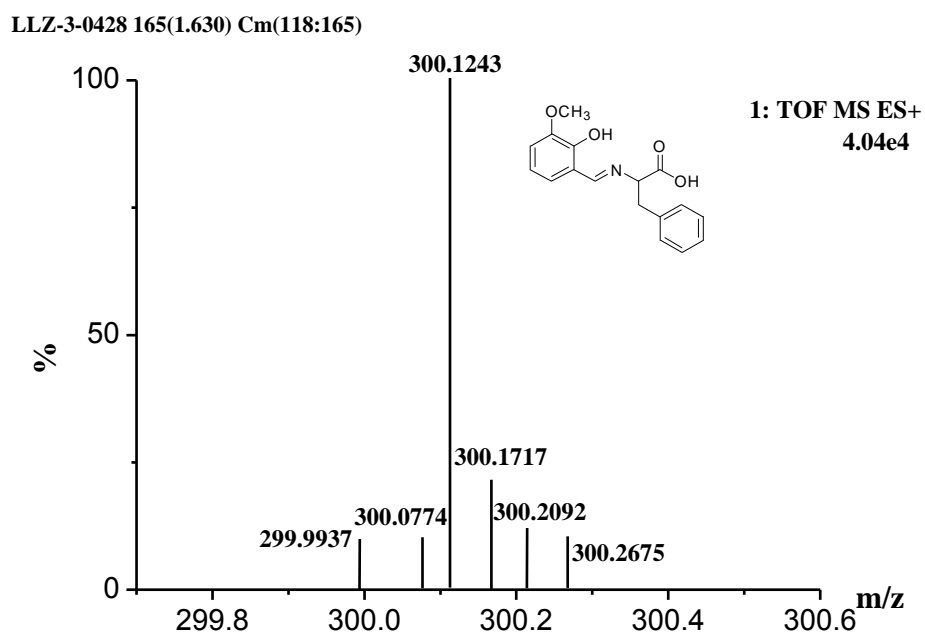
Fig. S1. Mass spectrum of the Schiff base 1

### Schiff base 2



**Fig. S2.** Mass spectrum of the Schiff base 2

### Schiff base 3



**Fig. S3.** Mass spectrum of the Schiff base 3

## 2. <sup>1</sup>H NMR spectra of the Schiff bases 1, 2 and 3

The <sup>1</sup>H NMR spectra of the Schiff bases **1**, **2** and **3** in dimethyl sulfoxide (DMSO-*d*<sub>6</sub>) were recorded on Varian 400 MHz spectrometer. <sup>1</sup>H NMR spectra of Schiff bases **1** (Fig. S4), **2** (Fig. S5) and **3** (Fig. S6) were assigned as follows.

Schiff base **1**:

δ: 14.30 (s, 1H, COOH), 8.09 (s, 1H, CH=N), 7.20 (t, *J*=7.6, 4H, ArH), 7.15 (d, *J*=6.8, 2H, ArH), 7.10 (t, *J*=7.0, 1H, ArH), 6.71 (d, *J*=8.1, 1H, ArH), 6.66 (t, *J*=7.4, 1H, ArH), 3.82 (dd, *J*=9.5, 3.9, 1H, CH), 3.28 (dd, *J*=13.8, 3.9, 1H, CH<sub>2</sub>), 2.92 (dd, *J*=13.8, 9.5, 1H, CH<sub>2</sub>).

Schiff base **2**:

δ: 13.46 (s, 1H, COOH), 8.36 (d, *J*=12.5, 1H, CH=N), 7.62 – 7.55 (m, 2H, ArH), 7.51 (d, *J*=7.4, 1H, ArH), 7.23 (d, *J*=17.7, 5H, ArH), 7.12 (s, 1H, ArH), 7.05 (t, *J*=7.3, 1H, ArH), 6.57 (d, *J*=9.4, 1H, ArH), 4.12 (s, 1H, CH), 2.96 – 2.83 (m, 1H, CH<sub>2</sub>).

Schiff base **3**:

δ: 14.23 (s, 1H, COOH), 7.95 (s, 1H, CH=N), 7.23 – 7.17 (m, 2H, ArH), 7.17 – 7.09 (m, 3H, ArH), 6.78 (d, *J*=6.4, 1H, ArH), 6.69 (dd, *J*=8.0, 1.4, 1H, ArH), 6.41 (t, *J*=7.8, 1H, ArH), 3.87 (d, *J*=9.1, 1H, CH), 3.70 (s, 3H, OCH<sub>3</sub>), 3.28 (dd, *J*=14.0, 3.8, 1H, CH<sub>2</sub>), 2.91 (dd, *J*=13.9, 9.7, 1H, CH<sub>2</sub>).

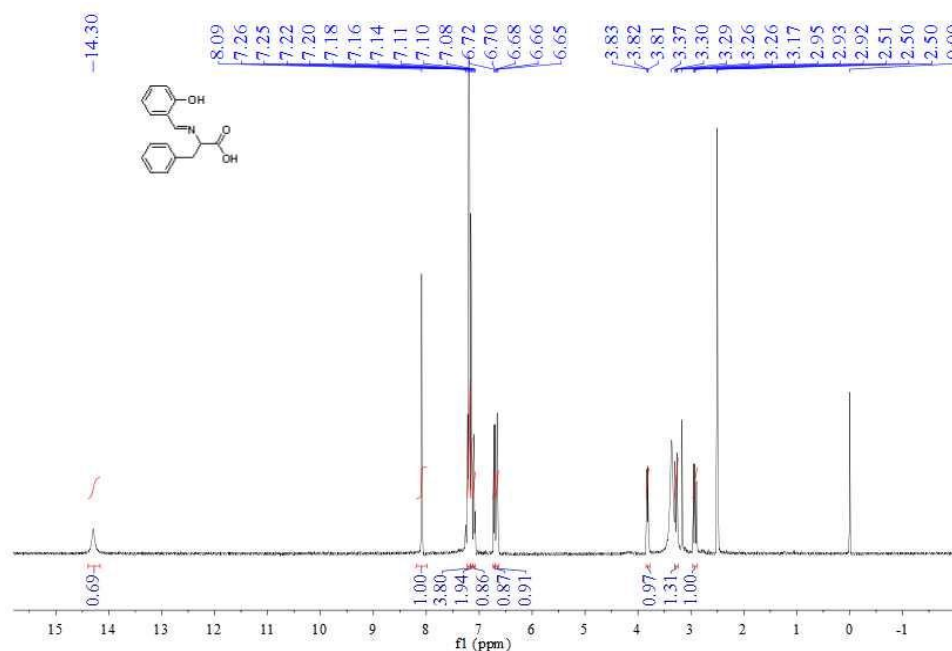
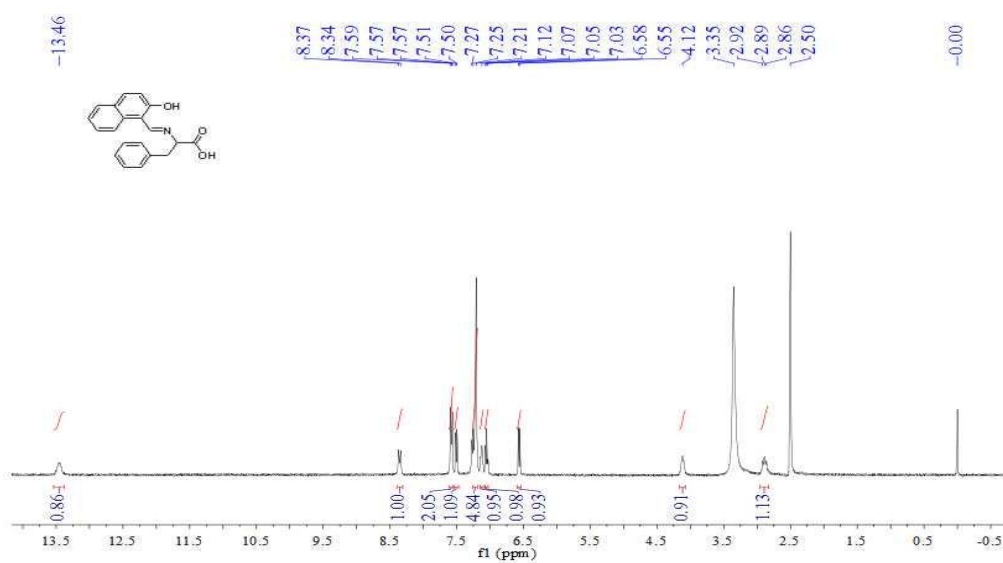
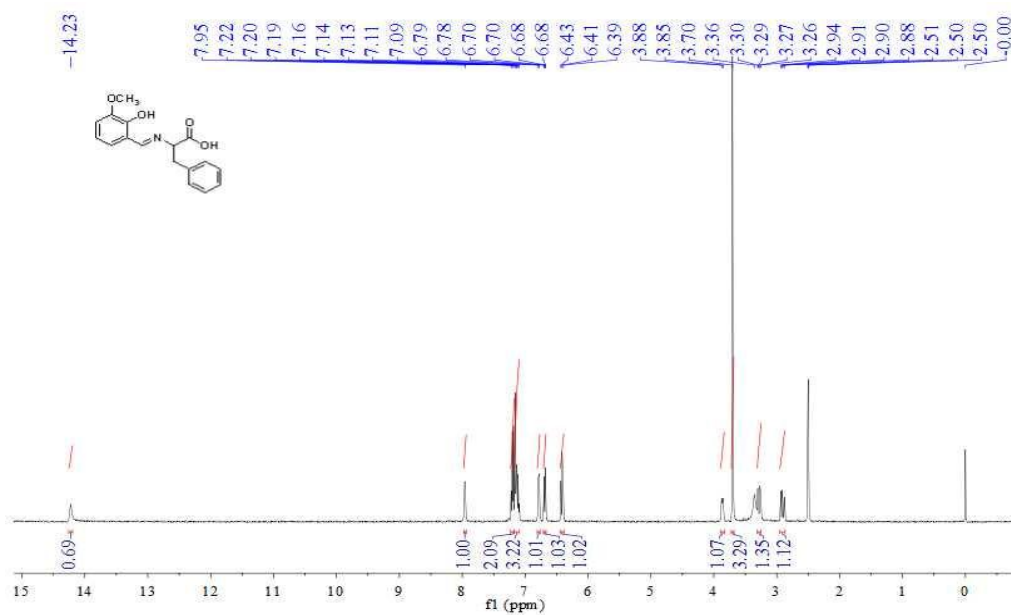


Fig. S4. <sup>1</sup>H NMR spectrum of the Schiff base **1**



**Fig. S5.**  $^1\text{H}$  NMR spectrum of the Schiff base 2



**Fig. S6.**  $^1\text{H}$  NMR spectrum of the Schiff base 3

### 3. CheckCIF/PLATON reports for the crystal structure determinations of the Complexes 1, 2 and 3

#### 3.1 Complex 1

##### checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.    CIF dictionary    Interpreting this report

##### Datablock: 131107e

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Bond precision:    C-C = 0.0062 A                      Wavelength=0.71073

Cell:                      a=26.741(3)            b=18.1651(17)            c=11.8350(9)  
                                    alpha=90                      beta=108.528(2)            gamma=90

Temperature:            298 K

	Calculated	Reported
Volume	5450.9(9)	5450.9(8)
Space group	C 2/c	C2/c
Hall group	-C 2yc	?
Moiety formula	C29 H25 N3 Ni O4, C H4 O	?
Sum formula	C30 H29 N3 Ni O5	C30 H29 N3 Ni O5
Mr	570.25	570.27
Dx,g cm-3	1.390	1.390
Z	8	8
Mu (mm-1)	0.756	0.756
F000	2384.0	2384.0
F000'	2387.64	
h,k,lmax	31,21,14	31,21,14
Nref	4824	4816
Tmin,Tmax	0.730,0.768	0.737,0.778
Tmin'	0.715	

Correction method= # Reported T Limits: Tmin=0.737 Tmax=0.778  
AbsCorr = MULTI-SCAN

Data completeness= 0.998                      Theta(max)= 25.020

R(reflections)= 0.0432( 3035)                      wR2(reflections)= 0.1248( 4816)

S = 1.094    Npar= 366

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The following ALERTS were generated. Each ALERT has the format  
test-name\_ALERT\_alert-type\_alert-level.  
Click on the hyperlinks for more details of the test.

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**Alert level C**

PLAT331\_ALERT\_2\_C Small Average Phenyl C-C Dist C4 -C9 1.37 Ang.  
PLAT341\_ALERT\_3\_C Low Bond Precision on C-C Bonds ..... 0.00625 Ang.  
PLAT480\_ALERT\_4\_C Long H...A H-Bond Reported H29A ..03 2.63 Ang.

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**Alert level G**

PLAT002\_ALERT\_2\_G Number of Distance or Angle Restraints on AtSite 4 Note  
PLAT005\_ALERT\_5\_G No Embedded Refinement Details Found in the CIF Please Do !  
PLAT007\_ALERT\_5\_G Number of Unrefined Donor-H Atoms ..... 3 Report  
PLAT083\_ALERT\_2\_G SHELXL Second Parameter in WGHT Unusually Large 5.89 Why ?  
PLAT093\_ALERT\_1\_G No s.u.'s on H-positions, Refinement Reported as mixed Check  
PLAT128\_ALERT\_4\_G Alternate Setting for Input Space Group C2/c I2/a Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 2 ) 100% Note  
PLAT302\_ALERT\_4\_G Anion/Solvent/Minor-Residue Disorder (Resd 3 ) 100% Note  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 2 3.17 Check  
PLAT304\_ALERT\_4\_G Non-Integer Number of Atoms in ..... Resd 3 2.83 Check  
PLAT720\_ALERT\_4\_G Number of Unusual/Non-Standard Labels ..... 1 Note  
PLAT793\_ALERT\_4\_G Model has Chirality at C2 (Centro SPGR) R Verify  
PLAT860\_ALERT\_3\_G Number of Least-Squares Restraints ..... 3 Note  
PLAT899\_ALERT\_4\_G SHELXL97 is Deprecated and Succeeded by SHELXL 2018 Note

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0 ALERT level A = Most likely a serious problem - resolve or explain  
0 ALERT level B = A potentially serious problem, consider carefully  
3 ALERT level C = Check. Ensure it is not caused by an omission or oversight  
14 ALERT level G = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
3 ALERT type 2 Indicator that the structure model may be wrong or deficient  
2 ALERT type 3 Indicator that the structure quality may be low  
9 ALERT type 4 Improvement, methodology, query or suggestion  
2 ALERT type 5 Informative message, check

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It is advisable to attempt to resolve as many as possible of the alerts in all categories. Often the minor alerts point to easily fixed oversights, errors and omissions in your CIF or refinement strategy, so attention to these fine details can be worthwhile. In order to resolve some of the more serious problems it may be necessary to carry out additional measurements or structure refinements. However, the purpose of your study may justify the reported deviations and the more serious of these should normally be commented upon in the discussion or experimental section of a paper or in the "special\_details" fields of the CIF. checkCIF was carefully designed to identify outliers and unusual parameters, but every test has its limitations and alerts that are not important in a particular case may appear. Conversely, the absence of alerts does not guarantee there are no aspects of the results needing attention. It is up to the individual to critically assess their own results and, if necessary, seek expert advice.

#### **Publication of your CIF in IUCr journals**

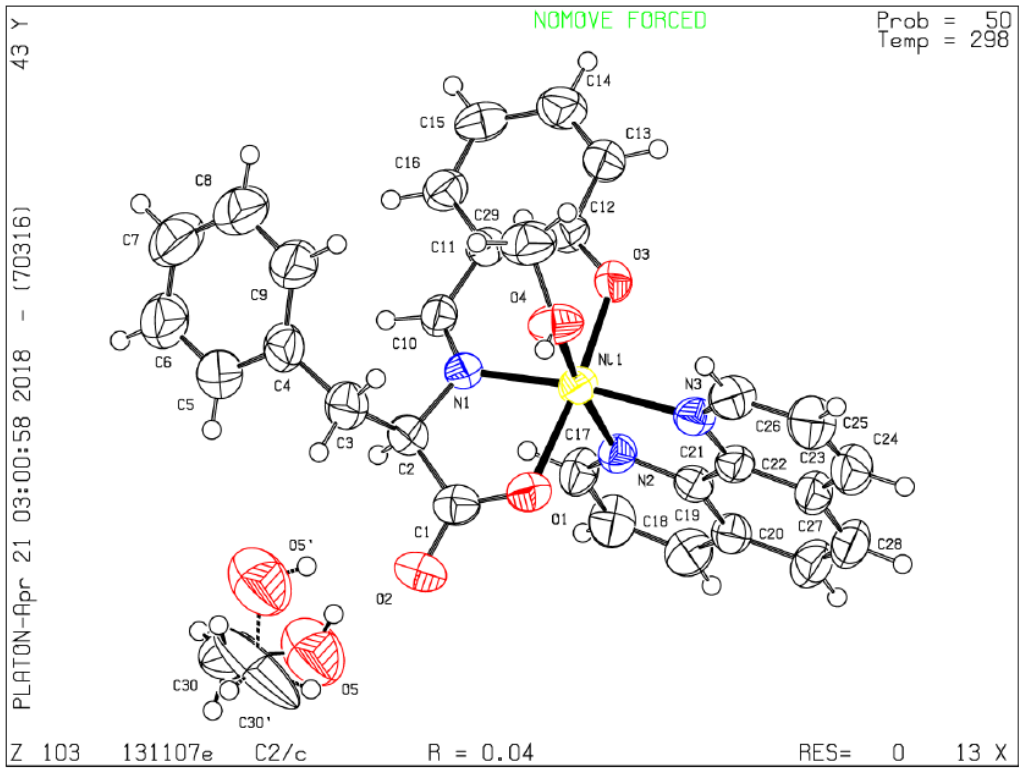
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

#### **Publication of your CIF in other journals**

Please refer to the *Notes for Authors* of the relevant journal for any special instructions relating to CIF submission.

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**





## 3.2 Complex 2

### checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.    CIF dictionary    Interpreting this report

### Datablock: 151211e

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Bond precision:    C-C = 0.0065 A                      Wavelength=0.71073

Cell:                      a=10.8240(8)                      b=11.9041(9)                      c=13.0879(11)  
                                    alpha=67.226(1)                      beta=73.566(2)                      gamma=64.094(1)  
Temperature:    298 K

	Calculated	Reported
Volume	1385.43(19)	1385.43(19)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C33 H27 N3 Ni O4	?
Sum formula	C33 H27 N3 Ni O4	C33 H27 N3 Ni O4
Mr	588.27	588.28
Dx, g cm-3	1.410	1.410
Z	2	2
Mu (mm-1)	0.744	0.744
F000	612.0	612.0
F000'	612.90	
h, k, lmax	12, 14, 15	12, 14, 15
Nref	4893	4791
Tmin, Tmax	0.843, 0.915	
Tmin'	0.843	

Correction method= Not given

Data completeness= 0.979                      Theta(max)= 25.015

R(reflections)= 0.0566( 3363)                      wR2(reflections)= 0.1456( 4791)

S = 0.952                                      Npar= 363

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The following ALERTS were generated. Each ALERT has the format  
**test-name\_ALERT\_alert-type\_alert-level**.  
Click on the hyperlinks for more details of the test.

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● **Alert level C**

```
PLAT018_ALERT_1_C_diffn_measured_fraction_theta_max .NE. *_full ! Check
PLAT094_ALERT_2_C Ratio of Maximum / Minimum Residual Density ... 2.20 Report
PLAT220_ALERT_2_C Non-Solvent Resd 1 C Ueq(max)/Ueq(min) Range 3.8 Ratio
PLAT234_ALERT_4_C Large Hirshfeld Difference C7 --C8 0.16 Ang.
PLAT241_ALERT_2_C High 'MainMol' Ueq as Compared to Neighbors of C7 Check
PLAT341_ALERT_3_C Low Bond Precision on C-C Bonds ..... 0.00645 Ang.
PLAT410_ALERT_2_C Short Intra H...H Contact H10 ..H17 1.98 Ang.
```

● **Alert level G**

```
PLAT793_ALERT_4_G Model has Chirality at C2 (Centro SPGR) S Verify
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0 **ALERT level A** = Most likely a serious problem - resolve or explain  
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7 **ALERT level C** = Check. Ensure it is not caused by an omission or oversight  
1 **ALERT level G** = General information/check it is not something unexpected

1 ALERT type 1 CIF construction/syntax error, inconsistent or missing data  
4 ALERT type 2 Indicator that the structure model may be wrong or deficient  
1 ALERT type 3 Indicator that the structure quality may be low  
2 ALERT type 4 Improvement, methodology, query or suggestion  
0 ALERT type 5 Informative message, check

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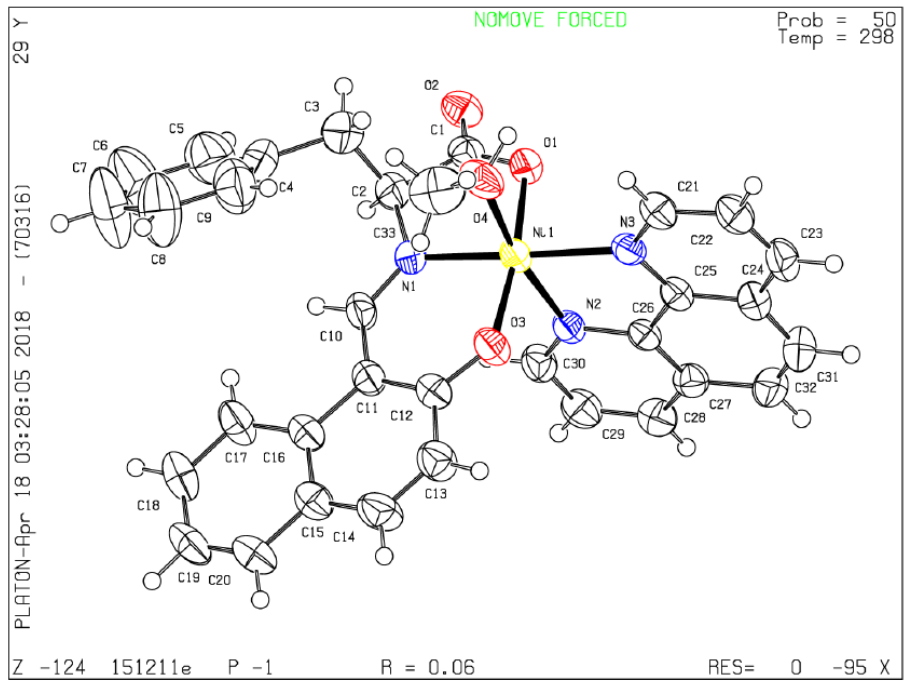
A basic structural check has been run on your CIF. These basic checks will be run on all CIFs submitted for publication in IUCr journals (*Acta Crystallographica*, *Journal of Applied Crystallography*, *Journal of Synchrotron Radiation*); however, if you intend to submit to *Acta Crystallographica Section C* or *E* or *IUCrData*, you should make sure that full publication checks are run on the final version of your CIF prior to submission.

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**PLATON version of 30/01/2018; check.def file version of 30/01/2018**



### 3.3 Complex 3

#### checkCIF/PLATON report

You have not supplied any structure factors. As a result the full set of tests cannot be run.

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No syntax errors found.      CIF dictionary      Interpreting this report

#### Datablock: 130323h

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Bond precision:    C-C = 0.0136 A                      Wavelength=0.71073

Cell:                      a=12.7068 (10)              b=13.5015 (14)              c=29.9214 (17)  
                                    alpha=83.667 (2)              beta=82.747 (1)              gamma=63.979 (1)  
Temperature:    293 K

	Calculated	Reported
Volume	4567.4 (6)	4567.4 (6)
Space group	P -1	P-1
Hall group	-P 1	?
Moiety formula	3 (C30 H27 N3 Ni O5), 5 (C H4 O)	?
Sum formula	C95 H101 N9 Ni3 O20	C95 H101 N9 Ni3 O20
Mr	1864.92	1864.98
Dx, g cm-3	1.356	1.356
Z	2	2
Mu (mm-1)	0.687	0.687
F000	1956.0	1956.0
F000'	1958.85	
h,k,lmax	15,16,35	15,16,35
Nref	16133	16112
Tmin,Tmax	0.842,0.884	0.847,0.886
Tmin'	0.842	

Correction method= # Reported T Limits: Tmin=0.847 Tmax=0.886  
AbsCorr = MULTI-SCAN

Data completeness= 0.999                      Theta(max)= 25.020

R(reflections)= 0.0870 ( 6748)              wR2(reflections)= 0.2584 ( 16112)

S = 1.004                                      Npar= 1155

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The following ALERTS were generated. Each ALERT has the format  
test-name ALERT\_alert-type\_alert-level.  
Click on the hyperlinks for more details of the test.

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● Alert level C

PLAT026_ALERT_3_C	Ratio Observed / Unique Reflections (too) Low ..	42%	Check
PLAT084_ALERT_3_C	High wR2 Value (i.e. > 0.25) .....	0.26	Report
PLAT220_ALERT_2_C	Non-Solvent Resd 3 C Ueq(max)/Ueq(min) Range	3.5	Ratio
PLAT230_ALERT_2_C	Hirshfeld Test Diff for O15 --C90 .	5.3	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C64 --C69 .	5.9	s.u.
PLAT230_ALERT_2_C	Hirshfeld Test Diff for C81 --C82 .	5.3	s.u.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C6 --C7	0.16	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C38 --C39	0.17	Ang.
PLAT234_ALERT_4_C	Large Hirshfeld Difference C62 --C63	0.16	Ang.
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C38	Check
PLAT241_ALERT_2_C	High 'MainMol' Ueq as Compared to Neighbors of	C66	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	09	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	014	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	015	Check
PLAT242_ALERT_2_C	Low 'MainMol' Ueq as Compared to Neighbors of	C64	Check
PLAT331_ALERT_2_C	Small Average Phenyl C-C Dist C34 -C39	1.37	Ang.
PLAT341_ALERT_3_C	Low Bond Precision on C-C Bonds .....	0.01364	Ang.

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● Alert level G

PLAT002_ALERT_2_G	Number of Distance or Angle Restraints on AtSite	30	Note
PLAT003_ALERT_2_G	Number of Uiso or Uij Restrained non-H Atoms ...	127	Report
PLAT005_ALERT_5_G	No Embedded Refinement Details Found in the CIF	Please Do !	
PLAT007_ALERT_5_G	Number of Unrefined Donor-H Atoms .....	8	Report
PLAT066_ALERT_1_G	Predicted and Reported Tmin&Tmax Range Identical	?	Check
PLAT199_ALERT_1_G	Reported _cell_measurement_temperature .... (K)	293	Check
PLAT200_ALERT_1_G	Reported _diffrn_ambient_temperature .... (K)	293	Check
PLAT793_ALERT_4_G	Model has Chirality at C2 (Centro SPGR)	R	Verify
PLAT793_ALERT_4_G	Model has Chirality at C32 (Centro SPGR)	S	Verify
PLAT793_ALERT_4_G	Model has Chirality at C62 (Centro SPGR)	R	Verify
PLAT860_ALERT_3_G	Number of Least-Squares Restraints .....	3688	Note
PLAT899_ALERT_4_G	SHELXL97 is Deprecated and Succeeded by SHELXL	2018	Note

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